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Elastic modulus of entangled polymers between cross-linkings

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架橋点で拘束された鎖の絡み合いを調べることにより、ゲルの弾性を解析をすることが本研究の目的である。ゲルにおいて鎖の絡まり合いを調べることは２つの効果の解明につながる。１つは架橋点間の鎖は絡まることで配位エントロピーが変わり弾性定数は減少する。２つめは膨潤過程や、外力による伸張において絡み合った鎖同士は一部のモノマーが極端に接近する。このときに鎖間ではL. J. 力などによる極端な斥力が働き膨潤、伸張を妨げる。結果としてゲル全体の弾性定数を上げ膨潤率を下げることになる。用いたモデルは、ランダムに分布させた架橋点をガウス鎖でつなぎネットワークを作った。この架橋点で拘束された鎖の弾性定数を求めている。

1 Introduction

A chemical gel is a polymer chain network that is chemically cross-linked and immersed in a good solvent. The network subjected to mechanical deformation. As long as the deformation does not break the chemical structure of the gel, the response will be determined by external conditions. The structure of the network is uniquely defined by fact that polymers joined to each cross-linked point and is fixed for all the time of the preparation of the gel. We refer to the state of preparation as the initial. The final state of the swollen and deformed network depends indirectly on the conditions of network preparation, since they determine the frozen structure.

The main motivation of the present simulation research is to study the elastic modulus of cross-linked polymer chain in the gels.

2 Simulation

We consider a gel model for NIPA gel consisting of two functional polymers and four functional cross-linings. Here we assume that two functional polymer correspond to poly N-isopropylacrylamide, and four-functional monomer to N-methylenebisacrylamide.

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First, we distribute randomly a large number of cross-linking on an assumed finite space. They are fixed on the initial point for all the time. Second, an end of a polymer is jointed to one cross-linking, and another end randomly move on the space and the end approach another cross-linking. We assume the reaction to occur only when monomers come within the radius of the cross-linking We neglect dangling ends assume that the network is formed by cross-linking very long chains above the gelation point. The model is the randomly cross-linked network[1]of Gaussian chains with no excluded volume. However, this simply model contain topological effect [2] which account for the existence of permanent entanglements in real network. Here, we change the cross-linked polymer for the ring polymer[3].

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